

Butyl butyrate
109-21-7 | DTXSID7041702

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 4.62 days

Global applicability domain: Outside

Local applicability domain index: 3.08e-01

Confidence level: 7.57e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>2-Methylheptane</div> <div>Measured: 12.5</div> <div>Predicted: 3.99</div>	<div>Image not found</div> <div>Tetradeca-1,13-diene</div> <div>Measured: 367</div> <div>Predicted: 8.69</div>	<div>Image not found</div> <div>2-Methylhexane</div> <div>Measured: 12.5</div> <div>Predicted: 5.54</div>
<div>Image not found</div> <div>2,4-Dimethylheptane</div> <div>Measured: 61.9</div> <div>Predicted: 4.29</div>		